1-Pentanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,5-undecafluoro-

2706-91-4 | DTXSID8062600

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 4.16

Global applicability domain: Inside

Local applicability domain index: 9.51e-01

Confidence level: 5.97e-01

Nearest Neighbors from the Training Set

Image not found
1-Pentanol
Measured: 4.69
Predicted: 4.17

Image not found
Piperidine
Measured: 4.04
Predicted: 4.32

Image not found
Isopentyl alcohol
Measured: 4.52
Predicted: 4.24

Image not found
Dipropylamine
Measured: 3.59
Predicted: 4.37

Image not found
Butylamine
Measured: 3.61
Predicted: 4.09